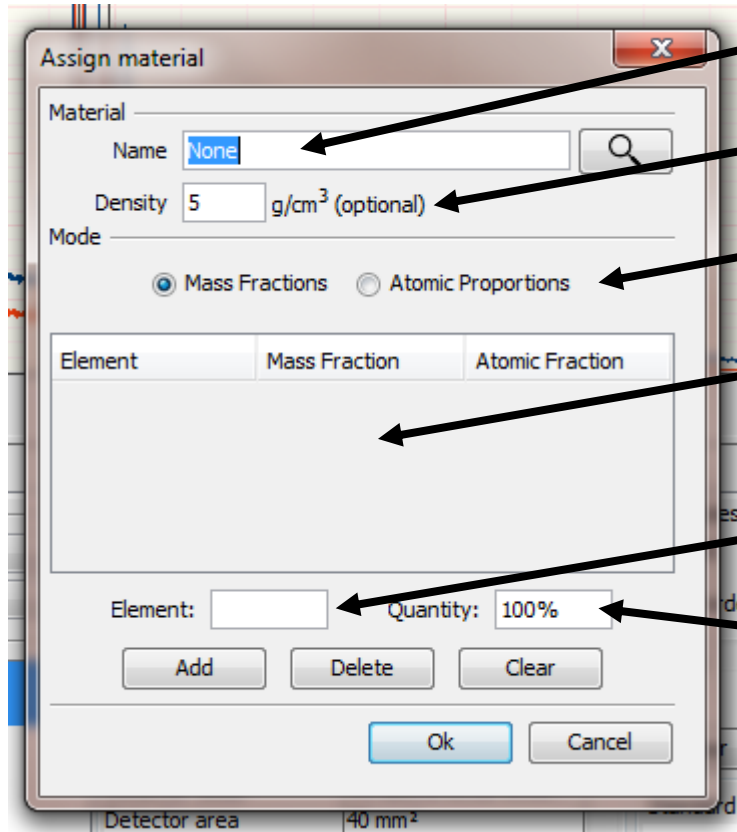


The Material Editor

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The tedious way...



The screenshot shows a software window titled "Assign material" with a close button (X) in the top right corner. The window contains the following fields and controls:

- Material Name:** A text box containing the word "None".
- Density:** A text box containing the number "5", followed by the unit "g/cm³ (optional)".
- Mode:** Two radio buttons: "Mass Fractions" (which is selected) and "Atomic Proportions".
- Table:** A table with three columns: "Element", "Mass Fraction", and "Atomic Fraction". The table is currently empty.
- Input Fields:** Below the table, there are two text boxes: "Element:" and "Quantity: 100%".
- Buttons:** Below the input fields are three buttons: "Add", "Delete", and "Clear". At the bottom of the window are "Ok" and "Cancel" buttons.

Annotations with arrows point to the following elements:

- Material Name: "None"
- Density: "5 g/cm³ (optional)"
- Mode: "Mass Fractions" radio button
- Table: The empty table structure
- Element input: "Element:" text box
- Quantity input: "Quantity: 100%" text box

A unique human friendly name

The density is required for Monte Carlo simulations

Input mode: mass fraction or atomic fraction

A table summarizing the amount of each element in the material definition.

The name, abbreviation or atomic number of the element to add.

The amount to add in mass percentage or atomic fraction

Tedious – mass fraction

Assign material

Material

Name

Density g/cm³ (optional)

Mode

☒ Mass Fractions ☐ Atomic Proportions

Element	Mass Fraction	Atomic Fraction
Magnesium	0.1166	0.1066
Aluminum	0.0491	0.0404
Silicon	0.2120	0.1678
Calcium	0.1090	0.0604
Iron	0.0774	0.0388

Element: Quantity:

Add 0.4276 mass fraction or 42.76 mass percent O.

Tedious – mass fraction

Assign material

Material

Name: None

Density: g/cm³ (optional)

Mode

☐ Mass Fractions ☒ Atomic Proportions

Element	Mass Fraction	Atomic Fraction
Aluminum	1.0000	2.0000

Element: Quantity:

Add Delete Clear

Ok Cancel

Add 3 atoms of O per
2 atoms of O

By chemical formula

Unambiguous chemical formulas entered here are parsed and the equivalent quantity of each element is entered.

Capitalization is critical. 'COP' is interpreted as 1 C atom, 1 O atom and 1 P atom while 'CoP' is interpreted as 1 Co atom and 1 P atom. 'CU' is C and U while 'Cu' is copper.

This formula is interpreted as 5 Ca atoms, 3 P atoms, 12 O atoms and 1 F atom. The braces '(' and ')' group the PO4 which is taken 3 times.

The parsing can be forced by pressing the

It is often a good idea to rename the material after entering a parse formula. I might name this one 'Fluorapatite'.

Assign material

Material

Name

Density g/cm³ (optional)

Mode

☒ Mass Fractions ☐ Atomic Proportions

Element	Mass Fraction	Atomic Fraction
Oxygen	0.3807	0.5714
Fluorine	0.0377	0.0476
Phosphorus	0.1843	0.1429
Calcium	0.3974	0.2381

Element: Quantity:

From the database

A material once entered is remembered.

DTSA-II builds a material database from the materials entered into the material editor. Whenever a name is entered into the 'Name' field, the program searches the database for previously defined materials with precisely that name. (Spelling and capitalization matter.)

The names "temp", "tmp", "crap", "junk", and "stuff" are neither stored nor retrieved.

The density is also stored in the database.

Assign material

Material

Name: Fluorapatite

Density: 3.15 g/cm³ (optional)

Mode: ☒ Mass Fractions ☐ Atomic Proportions

Element	Mass Fraction	Atomic Fraction
Oxygen	0.3807	0.5714
Fluorine	0.0377	0.0476
Phosphorus	0.1843	0.1429
Calcium	0.3974	0.2381

Element: Quantity: 100%

Add Delete Clear

Ok Cancel

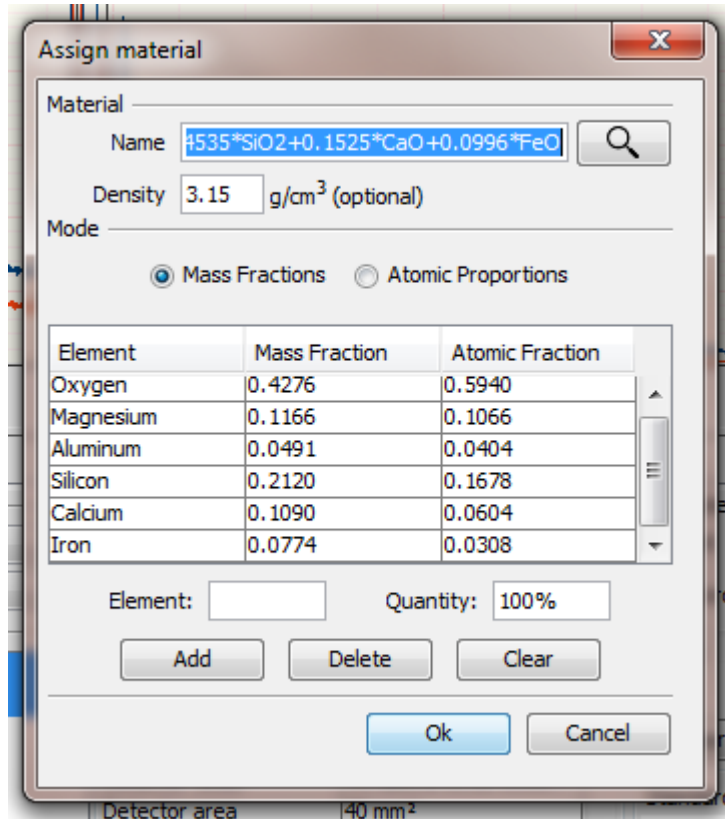
Advanced

Enter a sum of materials by mass-fraction.

For example: K412 glass is defined in terms of its oxide fractions as:

$0.1933 * \text{MgO} + 0.0927 * \text{Al}_2\text{O}_3 + 0.4535 * \text{SiO}_2 + 0.1525 * \text{CaO} + 0.0996 * \text{FeO}$

This is parsed as 0.1933 fraction by mass of MgO which is parsed as 1 atom of Mg and 1 atom of O plus 0.0927 fraction by mass of Al₂O₃ etc.



Remember a user-friendly name

When you click 'Ok', the dialog closes and the material is stored by name in the database.

If the name is easy-to-remember, you can recover the material definition from the database quickly and easily.